

# DSMC Shock Simulation of Saturn Entry Probe Conditions

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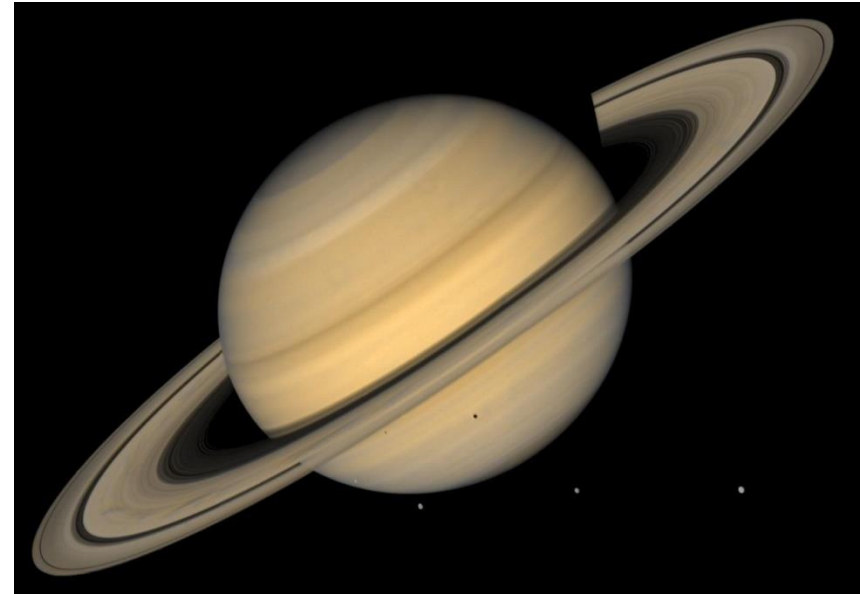
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- The 2013 Decadal Survey identified a probe mission to Saturn as a high priority.
- Saturn entry conditions:
  - High speed trajectories of ~25-29 km/s.
  - H<sub>2</sub>-He atmosphere mixture.
- Convective heating accounts for most of the total heat flux during entry.
- Significant uncertainty in the prediction of radiative heating.<sup>1</sup>



<sup>1</sup>Palmer, Prabhu, and Cruden, "Aeroheating Uncertainties in Uranus and Saturn Entries by the Monte Carlo Method"  
<http://nssdc.gsfc.nasa.gov/planetary/image/saturn.jpg>

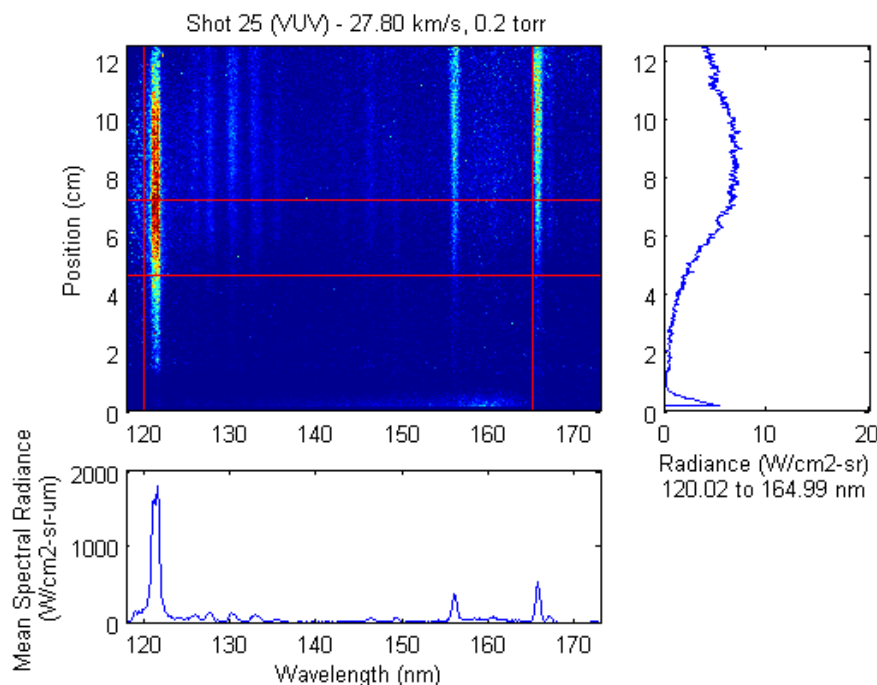
- Recent shock tube experiments of a  $\text{H}_2$ -He mixture have been performed in the NASA Ames Electric Arc Shock Tube (EAST)<sup>1</sup>.

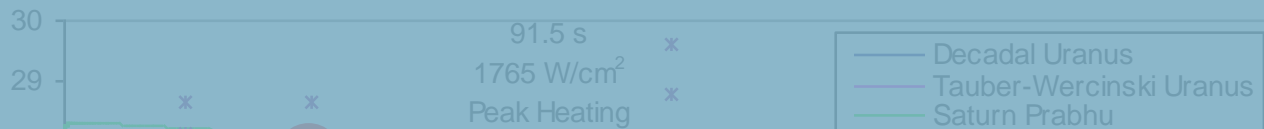
- Spectrometers measured emission in the VUV, UV, visible, and near-IR ranges.
- H and  $\text{H}_2$  emission measured.

- Observations

- Post-shock region did not equilibrate by 5 cm.
- An induction period occurred several cm behind shock.
- Radiance in the VUV range was observed in the pre-shock region indicating diffusion of hydrogen upstream of the shock.

27.8 km/s, 0.2 Torr, VUV range

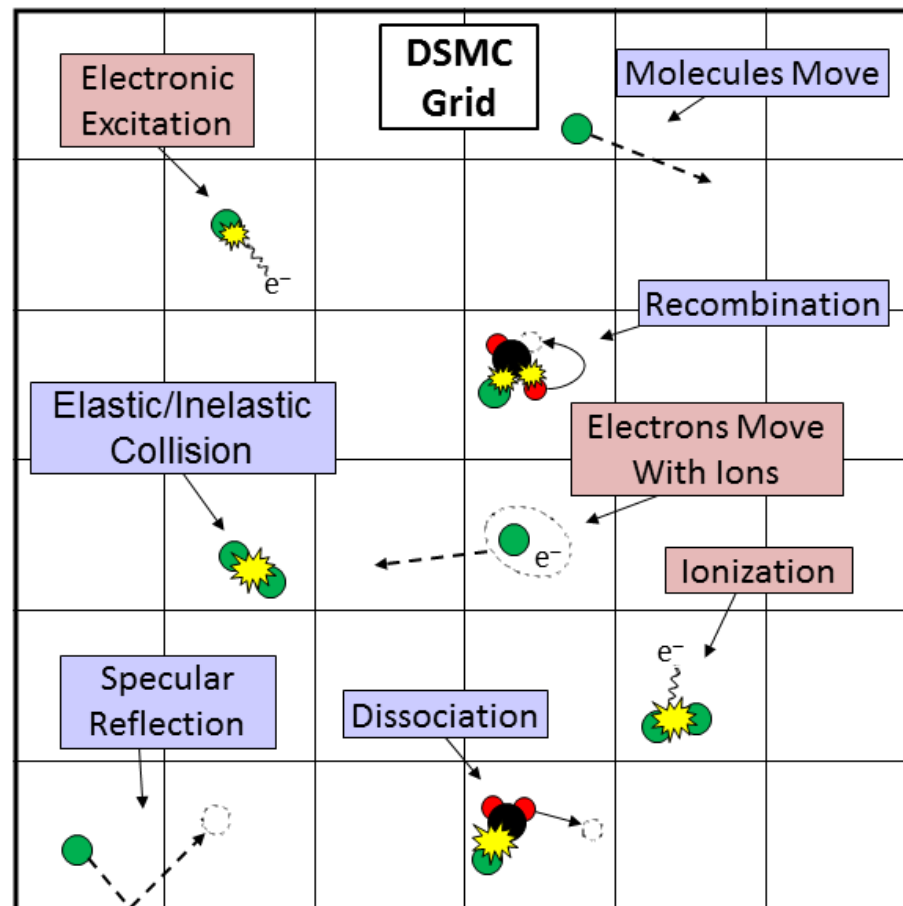




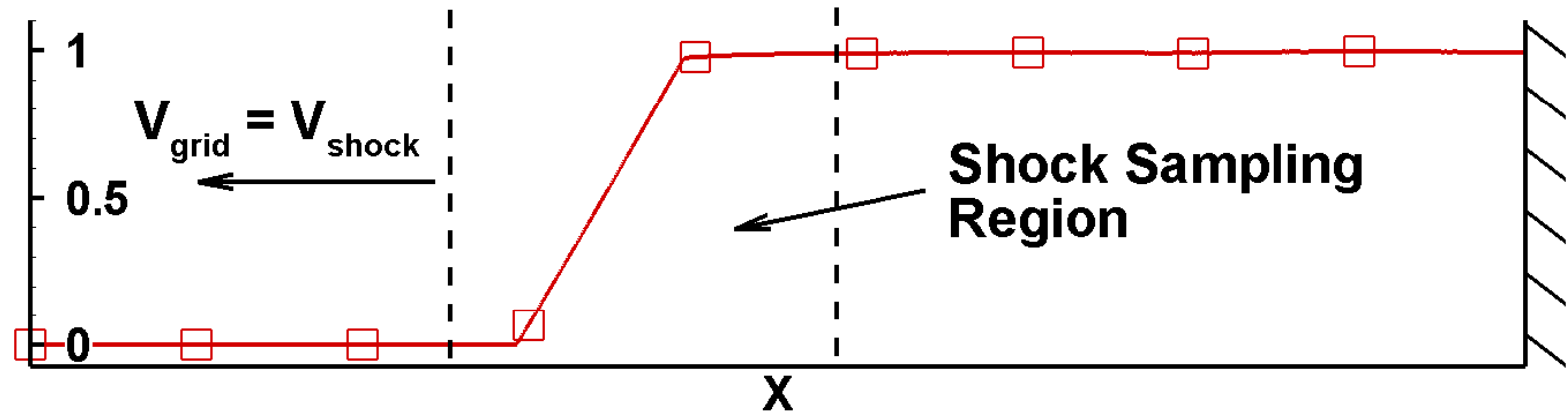
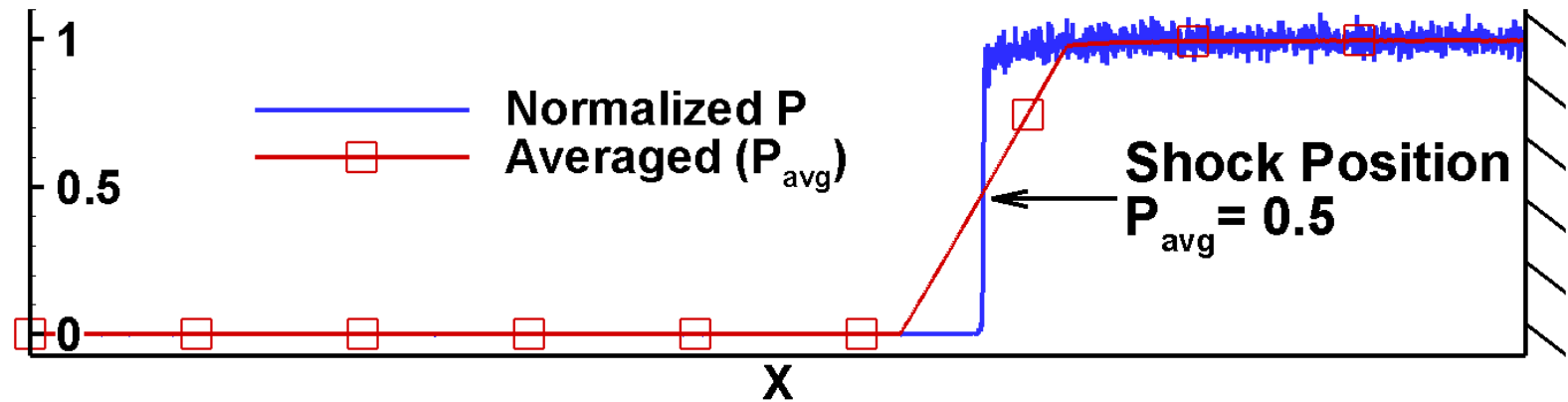
## Motivation:

- Investigate the influence of non-equilibrium phenomena on Saturn entry conditions.
- Identify physical mechanisms that explain the EAST experimental results.
  - Direct Simulation Monte Carlo (DSMC) method is required to model non-continuum features.
- Complete a first attempt of modeling a high temperature H<sub>2</sub>-He mixture with DSMC.
  - Develop high temperature parameters and identify areas requiring improvement.
- DSMC simulations of Shot 25 and Shot 17 are performed here.

- Stochastic model of individual particles and their physics.
  - Each DSMC 'particle' represents many real particles.
  - Can model large non-equilibrium regions.
- Probabilistic approach
  - Simplified models use cross sections and probabilities determined from experiments.
- Applicable for rarefied flows
  - $Kn = \lambda/D > 0.01$
  - Continuum breaks down.
    - Must use Boltzmann equation.



## 1-D Unsteady Shock Simulation:



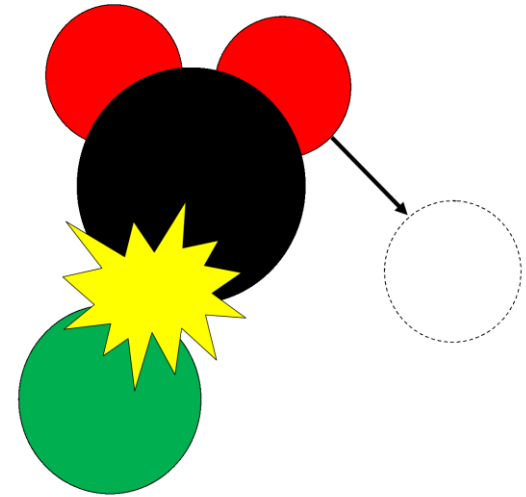
## Electronic Excitation Model:

- Model scheme follows previous work by Liechty.<sup>1</sup>
  - Post-collision energy transfer is performed with an acceptance-rejection procedure following Larsen-Borgnakke.
  - Electronic energy and degeneracy parameters for each electronic level are required.
- *Electronic* temperature is currently modeled as the *electron* temperature.
  - Free electron kinetic energy is the only component in the electronic temperature.
  - Equilibrates rapidly with the translational temperature.
  - Misrepresents the non-equilibrium in the heavy particle electronically excited states.

<sup>1</sup>Liechty, D. S., and Lewis, M. J., "Extension of the Quantum-kinetic Model to Lunar and Mars Return Physics"

## Collision Models:

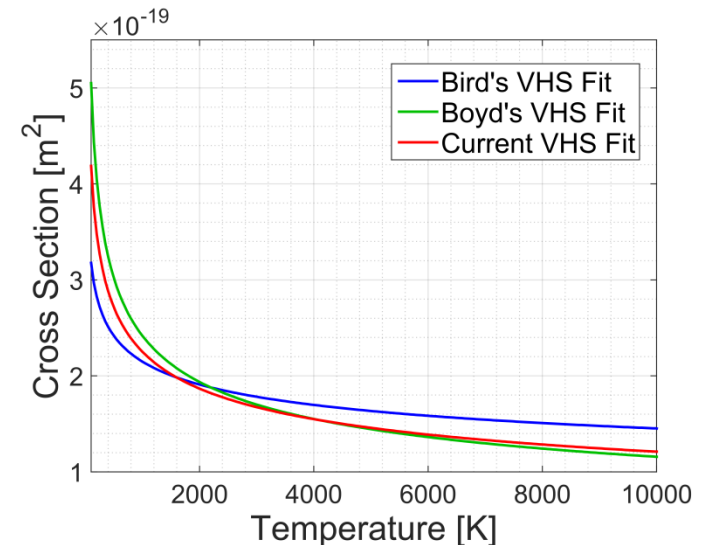
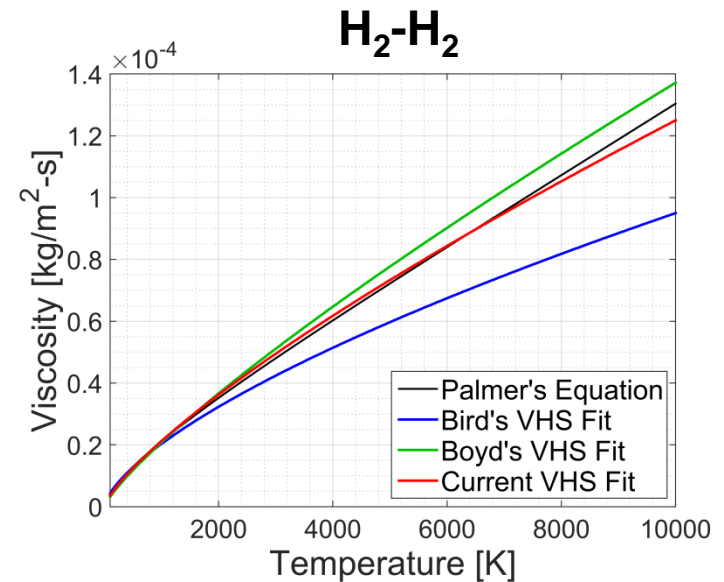
- Elastic collisions: Variable Hard Sphere (VHS)
  - Inelastic collisions: Larsen-Borgnakke
    - Rotational relaxation: Parker's model
    - Vibrational relaxation: Millikan-White
  - Chemical reactions: Total Collision Energy (TCE)
  - Quasi-neutrality: Free electrons travel with ions
- 
- From these models, over 50 input parameters are required for a 7-species  $\text{H}_2$ -He mixture ( $\text{H}_2$ , H, He,  $\text{H}_2^+$ ,  $\text{H}^+$ ,  $\text{He}^+$ ,  $\text{e}^-$ ).
    - Many of the DSMC parameters for  $\text{H}_2$ -He mixtures are outdated or unavailable in literature.
    - New or improved parameters were obtained when possible.





## VHS Parameters:

- Previous general VHS parameters were published by Bird<sup>1</sup> and Boyd<sup>2</sup>.
  - Collision partner independent.
  - Fit to low temperature data.
- Collision integrals provided by Palmer<sup>3</sup> were used to obtain high temperature VHS parameters.
- Species specific VHS parameters were curve fit for neutral-neutral and charge-neutral collisions.
- Charge-charge collision parameters were assumed to be identical to the charge-neutral parameters.
  - Necessary since the range of the VHS values is limited.
  - Introduces a small amount of error.



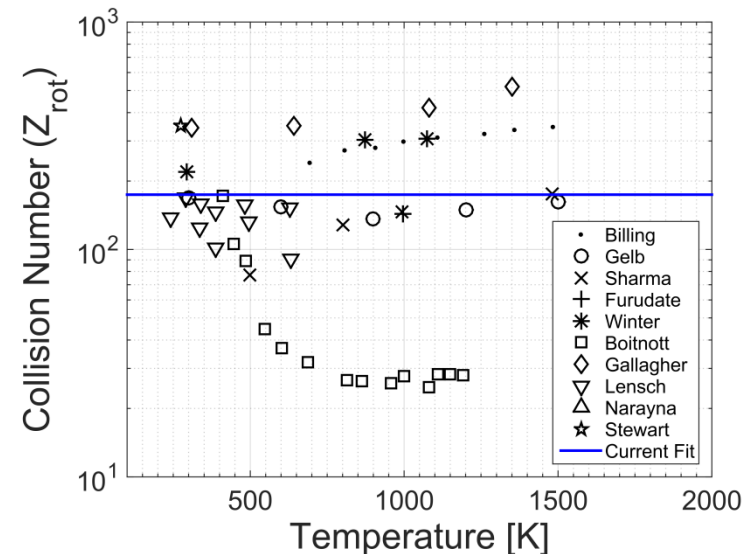
<sup>1</sup>G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*

<sup>2</sup>I.D. Boyd, "Monte Carlo Simulation of Nonequilibrium Flow in a Low-power Hydrogen Arcjet"

<sup>3</sup>Palmer, Prabhu, and Cruden, "Aeroheating Uncertainties in Uranus and Saturn Entries by the Monte Carlo Method"

## H<sub>2</sub> Relaxation Parameters:

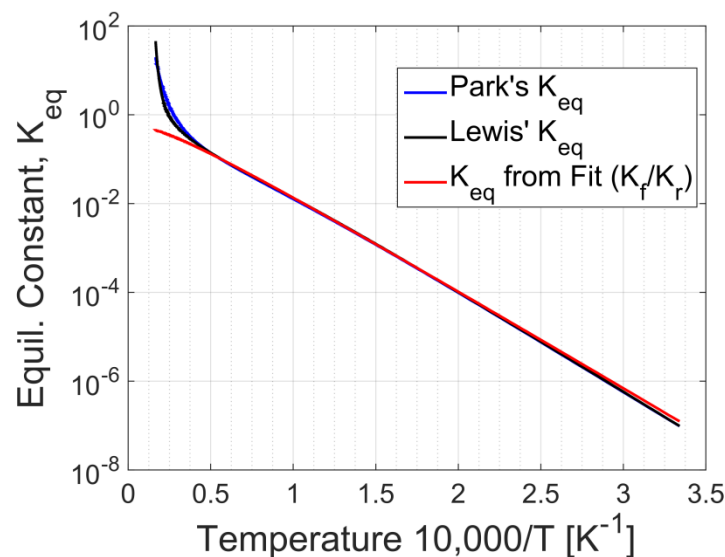
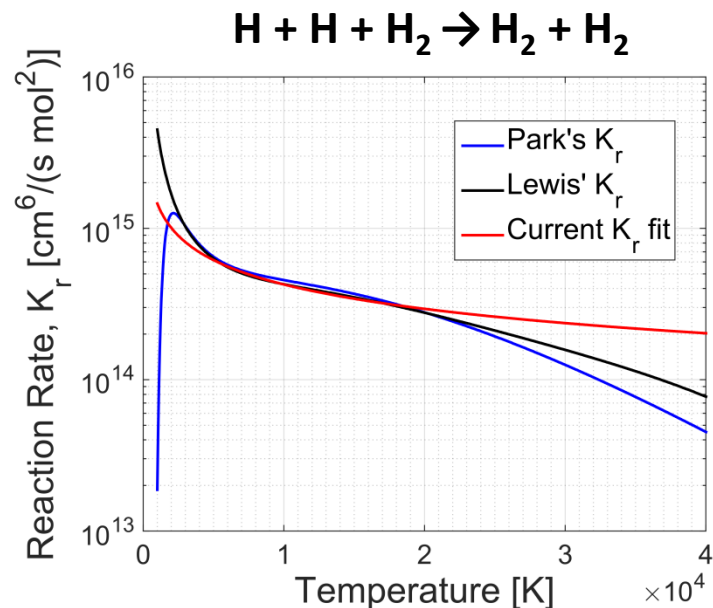
- Vibrational collision number is calculated from Millikan-White using Palmer's<sup>1</sup> parameters.
- A temperature dependent rotational collision number relationship is preferred (Parker).
  - H<sub>2</sub> is complex in rotation.
  - Compiled experimental data shows conflicting trends.
- Rotational collision number was "fit" to the data using a temperature independent value.
  - For a moderate temperature range between 200-1500 K, the fit was determined to be  $Z_{\text{rot}} = 174$ .



<sup>1</sup>Palmer, Prabhu, and Cruden, "Aeroheating Uncertainties in Uranus and Saturn Entries by the Monte Carlo Method"

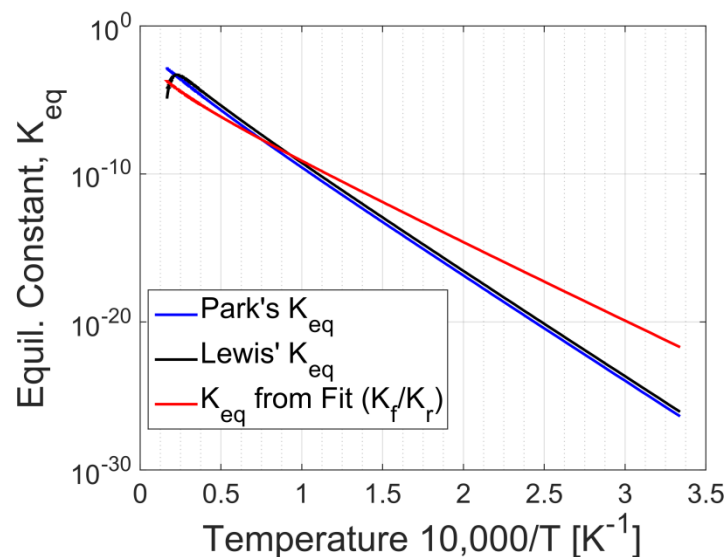
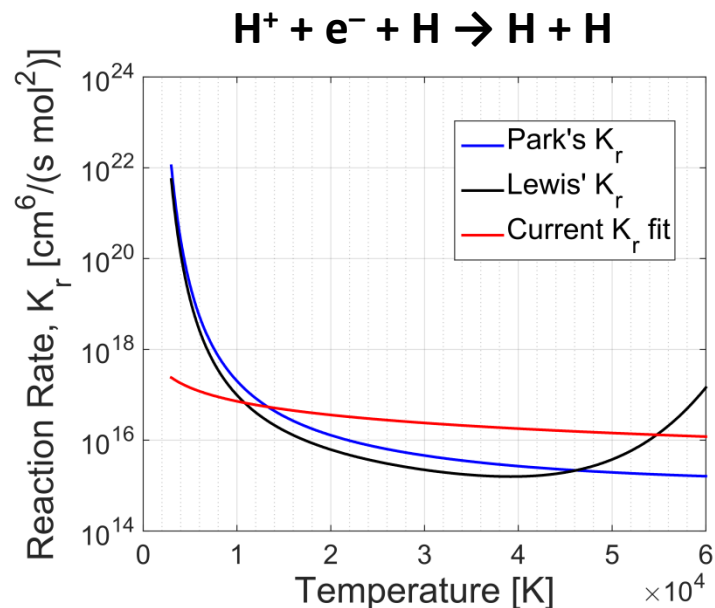
## Recombination Reaction Rates:

- Forward Arrhenius reaction rates ( $K_f$ ) were obtained from Leibowitz<sup>1</sup>.
- Reverse reaction rates ( $K_r$ ) were calculated from the equilibrium constant ( $K_{eq}$ ) and fit to an Arrhenius form.
  - Arrhenius fit is necessary for the TCE model.
- Neutral recombination reactions were fit to a temperature region between 5,000-20,000 K.
  - Over-predicts recombination at very high temperatures.
  - Under-predicts recombination at low temperatures.



## Recombination Reaction Rates:

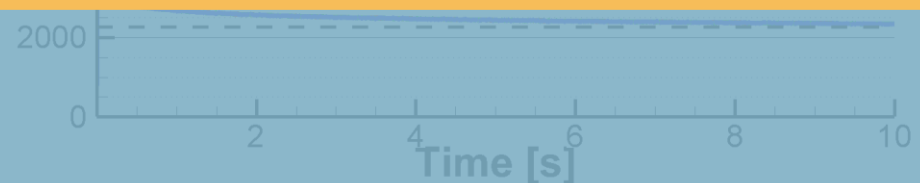
- Electron capture reaction rates are more difficult to curve fit.
  - Poor curve fits are due to constraints of the TCE model on the possible Arrhenius parameters.
- Large errors in the current electron capture rates are evident.
  - Over-predicts recombination at high temperatures.
  - Under-predicts recombination at low temperatures.
  - Leads to noticeable error in the equilibrium constant.



## How can we compare the DSMC results directly to the experimental data?



- Experiments measure radiative emission.
  - Must post-process DSMC results with a radiative solver.
- Simulate Shots 25 and 17.
  - Compare simulated results to experiments for the VUV, UV, visible, and near-IR ranges.
  - Identify models and parameters for future improvement.

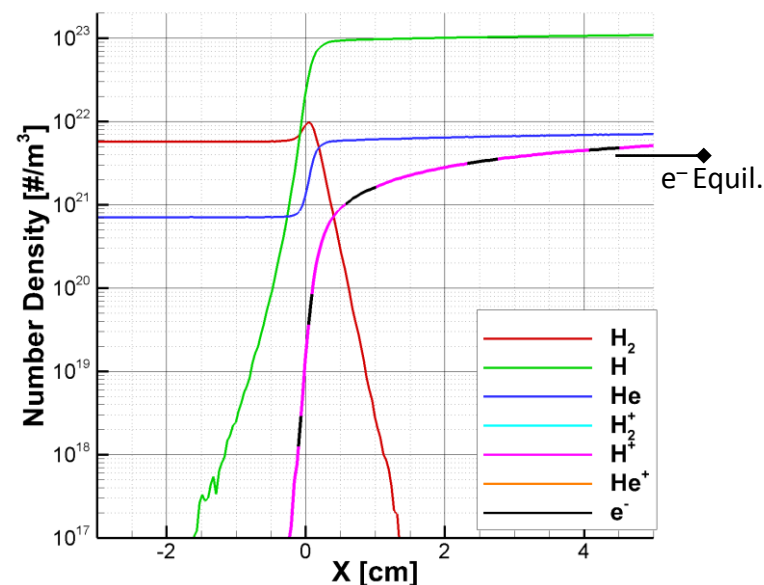
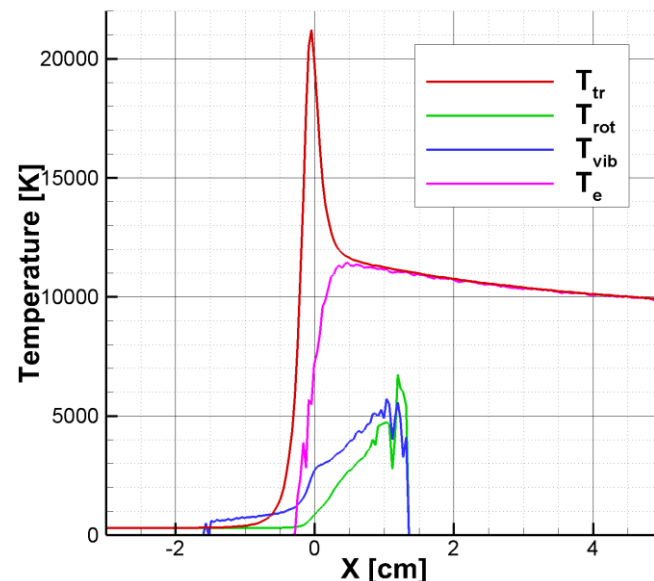


## NEQAIR:

- Line-by-line, tangent slab computation along a line of sight.
- Multiple spectral and spatial broadening mechanisms are accounted for.
- Instruments convolutions are applied to mimic experimental smearing.
- Number densities and temperatures are passed to NEQAIR.
  - Four temperature calculation ( $T_{tr}$ ,  $T_{rot}$ ,  $T_{vib}$ ,  $T_e$ ).
  - Currently, only a Boltzmann calculation for H is available.

## EAST Shot 25:

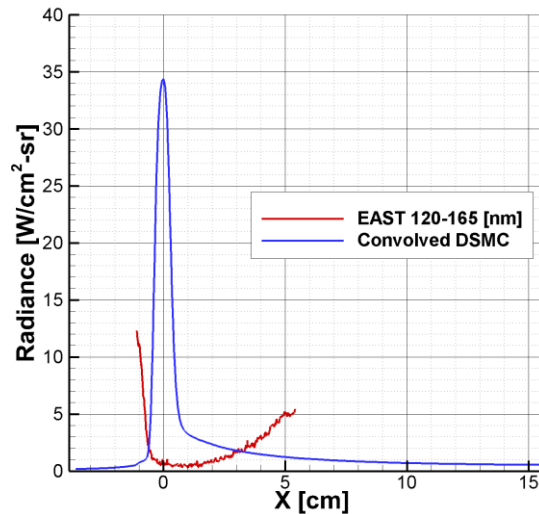
- Shock velocity: 27.8 km/s
- Initial pressure: 0.2 Torr
- Initial temperature: 300 K
- Freestream 89% H<sub>2</sub>: 11% He
- H<sub>2</sub> is dissociated by ~1.5 cm.
- H slightly diffuses upstream.
- Ionization begins immediately.
  - Degree of ionization is <10%.
  - Equilibrium has not been reached by 5 cm.
  - Higher electron number density than the experiment.
  - Expected equilibrium electron number density of  $4.2 \times 10^{21} \text{ m}^{-3}$ .



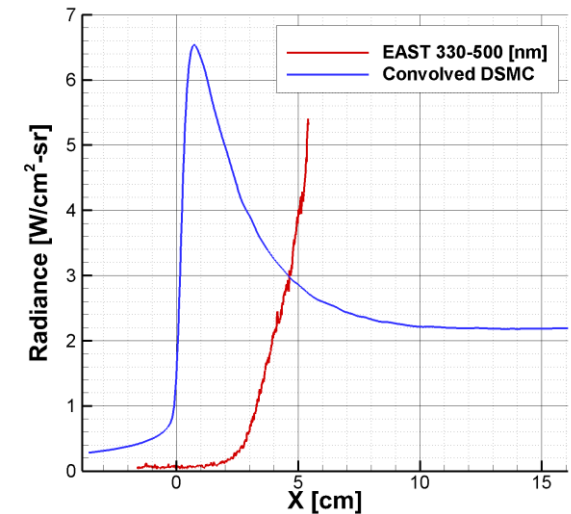
## NEQAIR Results:

- Radiance is generally over-predicted.
- Radiance measurements are roughly the correct shape.
- Molecular and Lyman- $\alpha$  emission occurs post-shock.
- Induction period is not seen in the simulation.

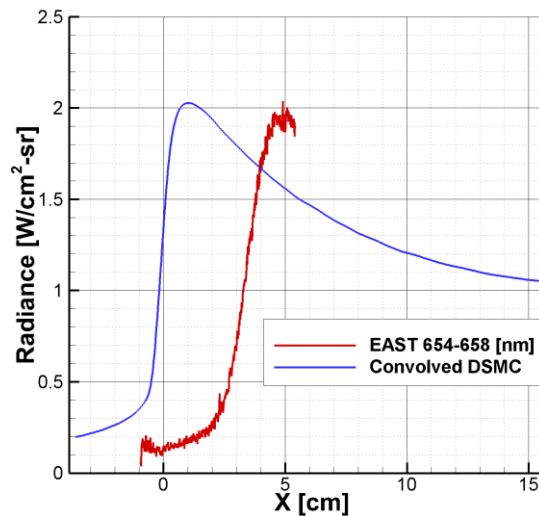
VUV



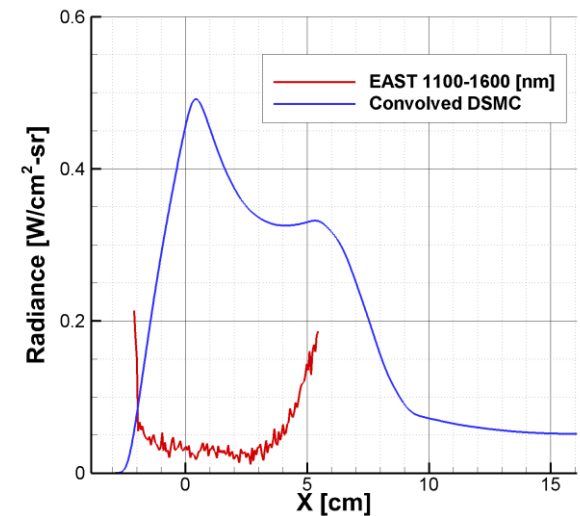
UV



Visible



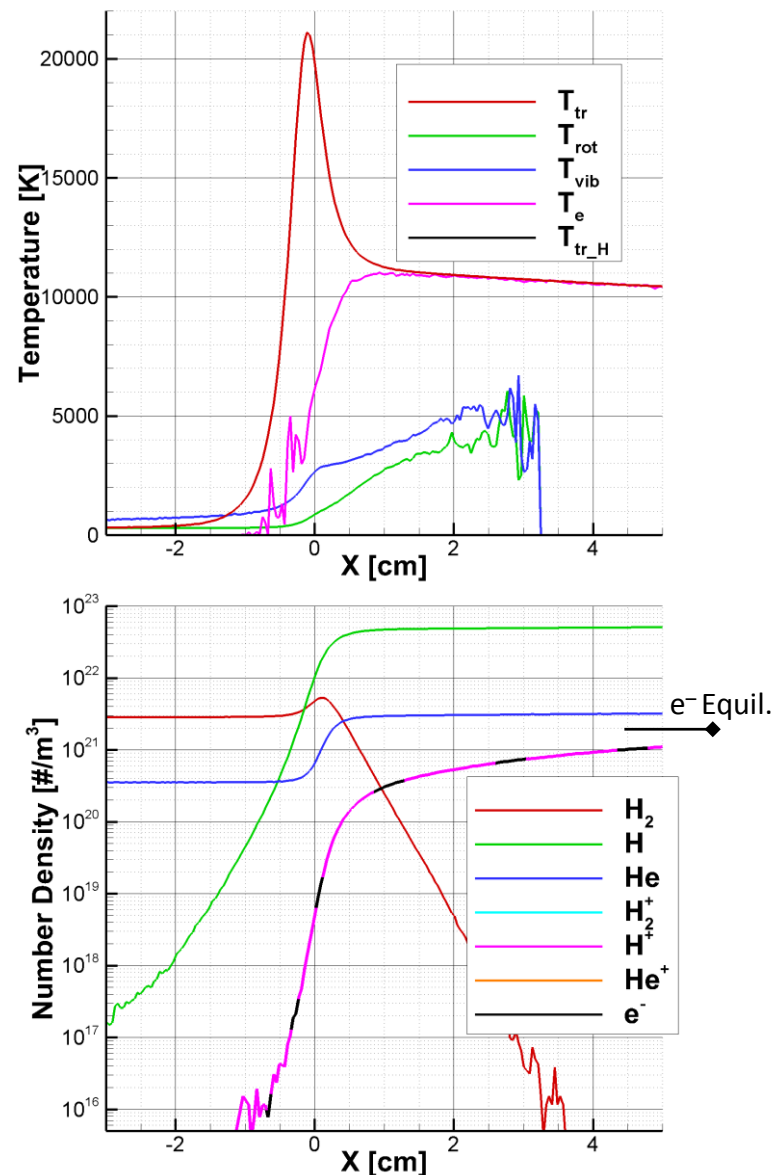
Near IR





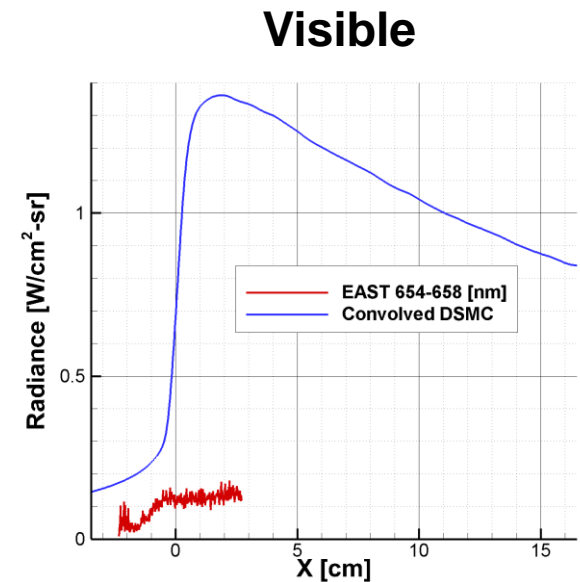
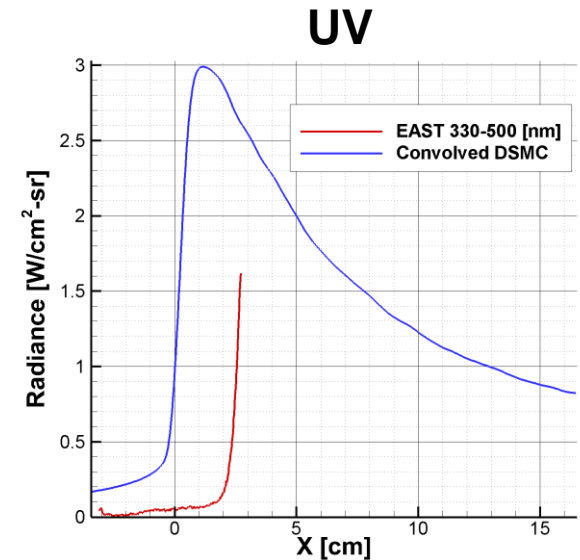
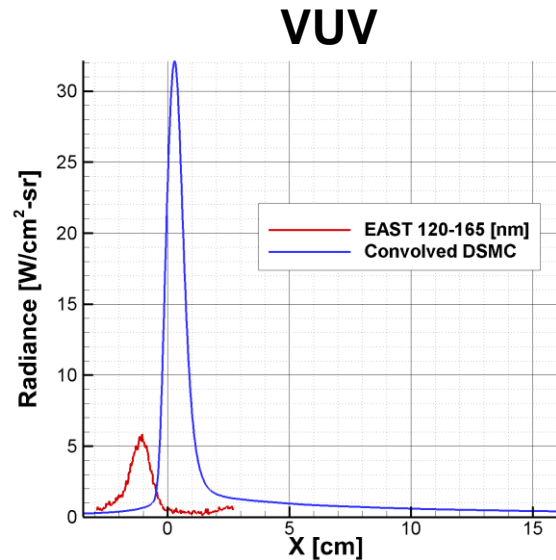
## EAST Shot 17:

- Shock velocity: 27.4 km/s
- Initial pressure: 0.1 Torr
- Initial temperature: 300 K
- Freestream 89% H<sub>2</sub>: 11% He
- H<sub>2</sub> persists more than twice the post-shock distance than Shot 25.
- H diffuses much further upstream.
- Equilibrium has not been reached by 5 cm.
  - Expected equilibrium electron number density of  $2.0 \times 10^{21} \text{ m}^{-3}$ .
  - Electron number density is trending towards this value, but still overshoots far downstream.



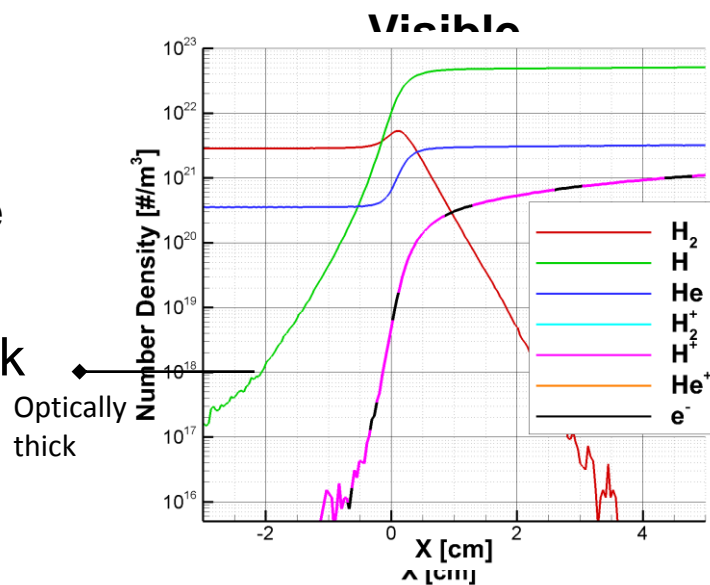
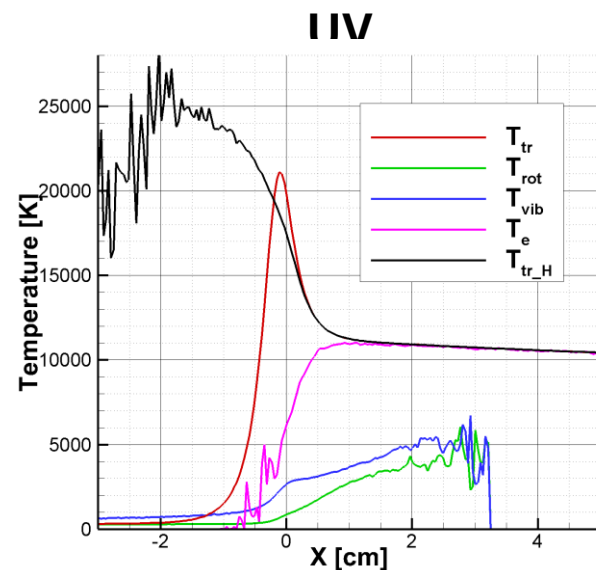
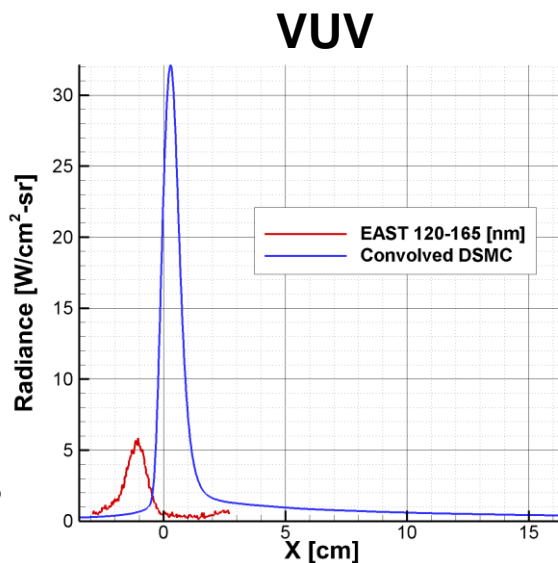
## NEQAIR Results:

- Similar comparisons as Shot 25.
- Radiance seems to take the correct shape.
- VUV radiance spike is approximately the correct width.
- Induction period is not seen in the UV range.
- Visible range radiance increase at the shock front for both.



## NEQAIR Results:

- NEQAIR radiation an electropresentation temperature to various zero upstream shock strengths.
- Ambipolar diffusion is not included in the DSMC model.
- Hot hydrogen diffuses upstream.
  - QSS rates for  $H(n=2 \rightarrow 1)$  should occur upstream.
  - NEQAIR
  - With the correct  $T_e$ , these particles should be
  - Terminated as the free electron kinetic
- Cruden<sup>1</sup> determined that H is optically thick as low as  $1.0 \times 10^{18} \text{ m}^{-3}$ .
  - Simulated H passes this value at the same location that the experimental radiance increase.



- An electronic excitation model was introduced to the DSMC code.
- High temperature DSMC parameters were obtained for a H<sub>2</sub>-He mixture.
- A 0-D relaxation was performed and the correct equilibrium was obtained.
- First attempts at simulating a non-equilibrium H<sub>2</sub>-He shock were completed and results were linked to the NEQAIR radiation solver.
  - Results were compared to the EAST experiments.
  - Non-equilibrium was confirmed with experiments to persist far downstream.
  - Atomic Hydrogen diffusion was observed upstream.
  - Simulated free electron number density was higher than the expected equilibrium values.
  - The ionization inductance period was not seen in the simulated radiance.
  - Simulated radiance was much higher than expected, but generally had the correct shape.

## High Priority:

- Formulate an improved representation of electronic temperature.
- Implement a more sophisticated chemical reaction model for recombination reactions in the DSMC code.
- Include quasi-steady state rates for H in NEQAIR.
- Perform a sensitivity analysis on the input parameters to identify the most important models and parameters that need improvements.

## Low Priority:

- Model ambipolar diffusion in the DSMC code.
- Obtain high temperature data for H<sub>2</sub> rotational relaxation and develop a temperature dependent equation.

## Conclusions:

- An electronic excitation model was introduced to the DSMC code.
- High temperature DSMC parameters were obtained for a H<sub>2</sub>-He mixture.
- A 0-D relaxation was performed and the correct equilibrium was obtained.
- First attempts at simulating a non-equilibrium H<sub>2</sub>-He shock were completed and results were linked to the NEQAIR radiation solver.
  - Results were compared to the EAST experiments.
  - Non-equilibrium was confirmed with experiments to persist far downstream.
  - Atomic Hydrogen diffusion was observed upstream.
  - Simulated free electron number density was higher than the expected equilibrium values.
  - The ionization inductance period was not seen in the simulated radiance.
  - Simulated radiance was much higher than expected, but generally had the correct shape.

# Questions?

## EAST Shot 25:

- Shock velocity: 27.8 km/s
- Initial pressure: 0.2 Torr
- Initial temperature: 300 K
- Freestream 89% H<sub>2</sub>: 11% He
- Comparison before (dashed) and after (solid) including an electronic excitation model.
- H slightly diffuses upstream.
- Ionization begins immediately
  - Electron number density increase by two orders of magnitude.
  - Equilibrium has not been reached by 5 cm.
  - Higher electron number density than the experiment.
  - Expected equilibrium electron number density of  $4.2 \times 10^{21} \text{ m}^{-3}$ .

